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Phonon scattering is treated only in the long wavelength limit. We have found that such and approximation is invalid in hot electron transport studies due to large momentum transfers involved. We are currently evaluating these rates from ab initio calculation. The results of this calculation are expected to include the effect of intervalley scattering mediated by LO and acoustic phonons more accurately. The analysis is completed, and computer evaluations of the result for several semiconductors are in process. This may change some of our quantitative conclusions.

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SEMICONDUCTOR ENGINEERING FOR HIGH-SPEED DEVICES

Quarterly R&D Status Report No.7

Covering the Period 16 December 1986 to 14 March 1987

27 April 1987

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I DESCRIPTION OF PROGRESS

This report summarizes major accomplishments during the period 16 December 1986 to March 1987.

For the first time, the calculated full tight-binding band structure is used in an accurate evaluation of scattering rates due to impurity and LO phonon scattering. These rates have been used in ballistic transport studies to obtain the mean free path of electrons at room temperature. There has been no change in the qualitative and quantitative conclusions drawn in our previous report (Report 6). The current status of our work is summarized in the enclosed preprint entitled "Semiconductor Alloys for High-Speed Electronics."

In general, phonon scattering is treated only in the long wavelength limit. We have found that such an approximation is invalid in hot electron transport studies due to large momentum transfers involved. We are currently evaluating these rates from *ab initio* calculation. The results of this calculation are expected to include the effect of intervalley scattering mediated by LO and acoustic phonons more accurately. The analysis is completed, and computer evaluations of the result for several semiconductors are in progress. This may change some of our quantitative conclusions.

In the materials considered here, the base region is doped with 10^{18} impurities per cm^3. This doping level is large enough to study the effect of electron-electron scattering on the transport properties. By assuming that electrons interact with other electrons through plasmons, we will include electron-electron scattering into our ballistic and drift transport studies.

We are also extending our evaluation to II-VI compounds and their alloys. The group velocity and mean free path of CdTe, ZnTe, and $Hg_{1-x}Cd_xTe$ for $x > 0.2$ where the material is a semiconductor are currently being generated. The results will be incorporated into a paper by May 15, 1987, to meet the deadline for the upcoming II-VI conference.

The transport calculations reported so far were carried out with a drifted-Maxwellian distribution for conduction electrons. A computer program that incorporates the Rees alogrithm for solving the Boltzmann equation in a self-consistent procedure, using an effective mass band structure, has been written. We still must modify this program to include our realistic calculated band structures and scattering rates.

II EQUIPMENT PURCHASED OR CONSTRUCTED

None

III TRIPS, MEETINGS, PAPERS, AND VISITS

(1) An-Ban Chen attended the March meeting of the APS in New York.

(2) A paper entitled "Hot Electron Transport in Semiconductor Alloys" was presented at the March meeting of the APS.

(3) A paper entitled "Semiconductor Alloys for High-Speed Electronics" will be published in the June issue of the proceedings of Society for the Advancement of Material and Processing Engineering (SAMPE).

IV PROBLEMS OR AREAS OF CONCERN

We have used up all but two hours of CRAY time allotted to us. Because the calculations to be carried out involve extensive use of computers, we request that another 25 hours of CRAY time be allotted to us for the year 1987-88.

V DEVIATION FROM PLANNED EFFORT

None

VI FISCAL STATUS

The total contract funding for the three-year period is $611,296. In the first year, $192,000 was spent. During the third quarter of year two (December 1, 1986 to February 28, 1987), $50,000 was spent.

SEMICONDUCTOR ALLOYS FOR HIGH-SPEED ELECTRONICS

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Abstract

The electron drift velocity, V, in semiconductors increase nonlinearly under the influence of applied electric fields to reach a peak value, V_p, at a threshold field, $\mathcal{E}_{V_{dp}}$; any further increase in electric field results in reduced v, giving rise to a negative differential resistance. High-speed device applications benefit from materials with maximum V_p and minimum $\mathcal{E}_{V_{dp}}$. By assuming a drifted Maxwellian distribution for electrons, we examine the effect of realistic band structure and scattering due to alloy, optical phonons, acoustic phonons and ionized impurities on the velocity-field characteristics. Calculations suggest InPAs, InPSb and GaInAs alloys have distinct advantage over the most favorable pure compounds (GaAs, InP and InAs). A review of experimental results and more accurate theoretical methods will be discussed.

Knowledge of variation of electron group velocity and scattering time as a function of injected electron energy is essential in designing ballistic transport devices. Effect of band structures and above mentioned scattering mechanisms on device length and injection angle will be discussed. We conclude that GaAs, InP and InAs have about equally high group velocities, and no alloy has an appreciably higher group velocity than these compounds. Also, the electrons injected in (100) direction have larger group velocity.

1. INTRODUCTION

Many compound semiconductors, notably GaAs and InP, have higher electron mobilities than Si and therefore are potentially superior materials for high speed devices. In this paper we shall examine the question of which semiconductor alloys are likely to prove to be optimum for various high speed applications. We shall break our discussion into two classes of devices, those whose active regions are sufficiently long so the carriers make many collisions as they transport across the device (drift transport)[1]; and those devices that are small enough so the carriers experience no collisions in the active region (ballistic transport) (2).

There are several features that distinguish this work from prior efforts. We are treating the electron motion based on realistic band structures rather than using the often-employed electron mass approximation (EMA), in which each valley is approximated by a parabolic band. To do this in the alloys of the form $A_{1-x}B_xC$ the band structures and alloy contribution to the scattering rate are calculated in the coherent potential approximation (CPA)[3].

The AC and BC compound band structures are fit to experiments; and CPA, a strong scattering theory, serves as an accurate interpolation method yielding the alloy band structures and scattering rates. This procedure is a well established theory whose errors can be estimated. Unlike the Monte Carlo method [4], which is also strong scattering theory, CPA automatically includes scattering-induced band shifts (the real part of the self energy) in the theory. These shifts modify the band structures and group velocities, and introduce significant deviations into the upper reaches of the conduction band structures occupied in hot electron transport. Moreover, the use of realistic band structures rather than EMA also causes quantitative changes in the electron-phonon, impurity, and electron scattering rates. All these efforts will be discussed in the oral presentation.

2. BALLISTIC TRANSPORT DEVICES

While drift transport devices are more common and certainly predate ballistic transport devices, the physics of their operation is more easily presented in reverse historical order. The conduction band electronic structures of several compounds are shown in Fig. 1. Their conduction band edges have been aligned to facilitate comparison. The corresponding group velocity

$$\vec{V}_g(\vec{k}) = \frac{1}{h}\nabla_{\vec{k}}\epsilon(\vec{k})$$

magnitude for these materials are presented in Fig. 2. In one class of diode devices[2] electrons are injected into the active region in a given direction and with a given energy. They then transport through the active, essentially field free, region to a collector. There are three important materials characteristics that determine device function.

1) The boundary conditions at the edges of the active region which determine the injection and collection efficiencies.

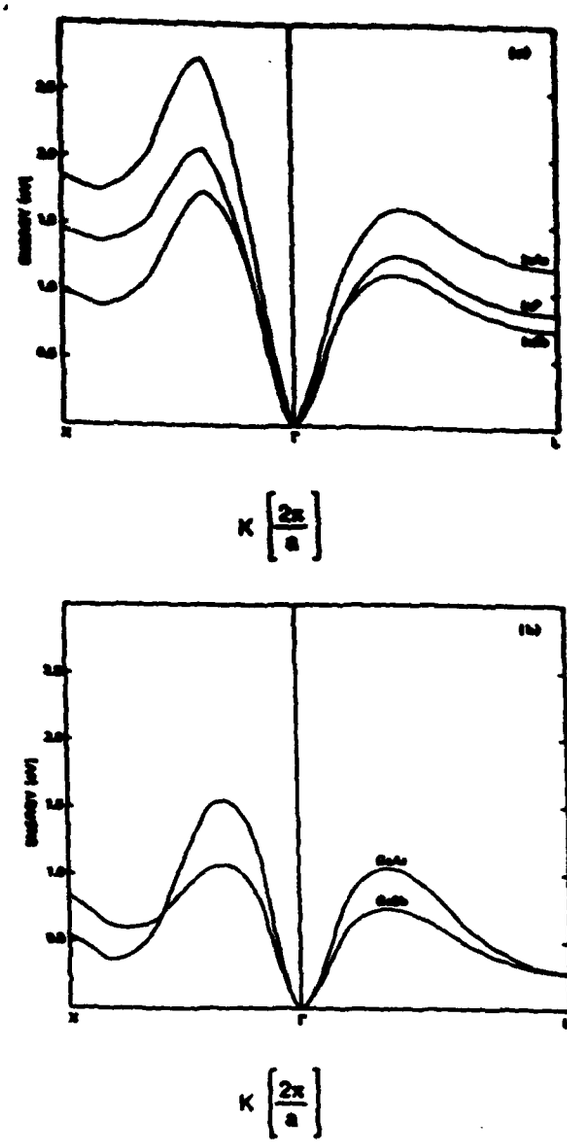

Fig. 1 The conduction band energies versus wave number for several compounds in the X and L directions. The reference energy for each curve is the conduction band edge.

2) The group velocity V_g for the injection conditions which along with the length of the active region, L, limits the response time.

3) The mean free path for the injection conditions which limits the size of the device if it is to function in the ballistic mode.

Since we are treating only bulk-like properties at present, we will not

Fig. 2 Group velocity versus wave number for several compounds and alloys.

examine the boundary conditions. There are generally lower limits to the feature size of the active region that one can build. The objective is to determine which material has the largest V_g and satisfies the condition $\lambda > L$.

The conduction band structures for the favorable materials all have their lowest energy at the central valley minimum near the zone center, called the Γ point. There are also satellite valleys with their minimum in the X (100) and L (111) directions. Most often the L minimum lies below the X minimum. From Fig. 2 one sees that the group velocities of electrons injected in the X direction are generally higher than those in the L direction and, it turns out, higher than in any other direction as well. As the injection energy increases the group velocity reaches a peak V_{gp} at the energy in the band structure $\epsilon_{V_{gp}}$ where the curvature changes sign, i.e. the effective mass changes sign. Clearly there is no advantage to be gained by injecting at a higher energy than $\epsilon_{V_{gp}}$.

There are often phenomena that limit practical injection energies to values well below $\epsilon_{V_{gp}}$. For example if ϵ exceeds the bandgap ϵ_g then the electrons can scatter by creating an electron-hole pair, which can limit λ to small values. If the minimum energy (referenced to zero at the conduction band edge) of the L satellite valley ϵ_L lies below $\epsilon_{V_{gp}}$, which is true for all cases we have examined, then electrons injected at energies $\epsilon > \epsilon_L$ experience additional interband scattering mediated by phonons, plasmons, impurities and alloy disorder that can greatly reduce their mean free path. In Fig. 3 the velocity scattering rates τ^{-1} for electrons injected into the (100) direction of GaAs due to polar optical scattering and impurity scattering due to 10^{18} impurities/cm^3, along with the corresponding mean free paths, are shown for various injection energies.

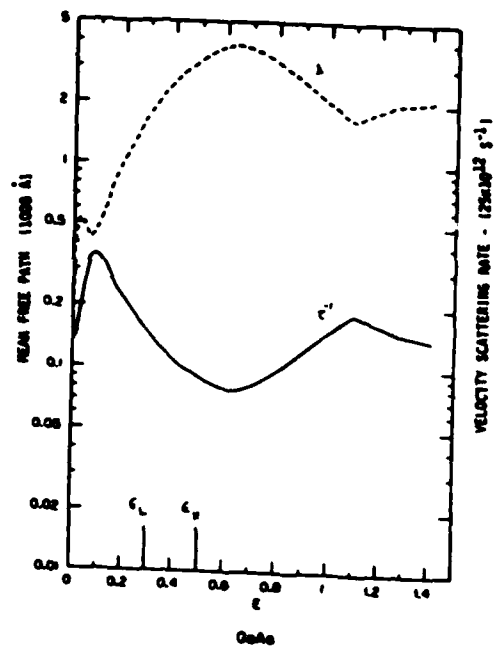

Fig. 3 The velocity scattering rate and the corresponding mean free path polar phonon and charged impurity (concentration 10^{18} cm^3) scattering in GaAs.

The energies ϵ_L and ϵ_X are shown. Note that nothing dramatic happens to τ^{-1} at $\epsilon = \epsilon_L$. We believe this is due in part to our not having included electron-phonon scattering coupled through the deformation potential, so this curve is probably not

correct for $\epsilon > \epsilon_L$. However, we are still examining this situation. One expects ϵ will have to rise somewhat above ϵ_L before τ^{-1} exhibits a change since at ϵ_L the density of states in the L valley vanishes so the intervalley scattering rate will be small. Only after ϵ is somewhat above ϵ_L will the intervalley rate compete with the intravalley rate and cause λ to decrease. In Fig. 3 τ^{-1} does not begin to increase because of intervalley scattering until ϵ gets well above ϵ_L (and also ϵ_X). This is because the matrix element for polar optical phonon scattering is inversely proportional to the wave number change of the electron which is large for intervalley scattering. In addition, V_g is still increasing for ϵ above ϵ_L hence λ overshoots $\lambda(\epsilon_L)$. We expect this will continue even when other scattering mechanisms are included, but the extent of the overshoot will probably be somewhat smaller than shown here.

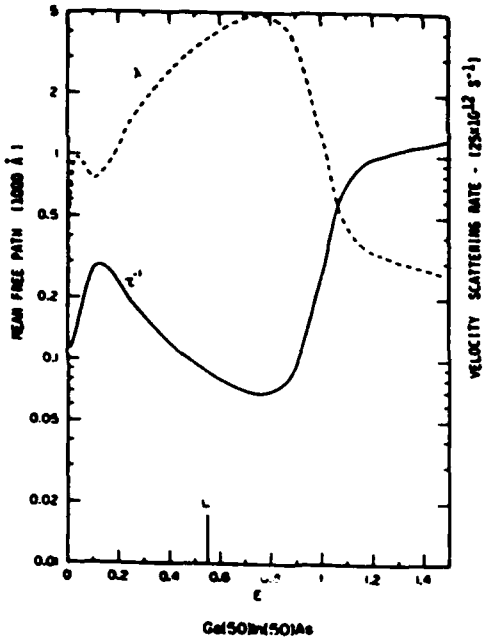

Fig. 4 The velocity scattering rate and the corresponding mean free path due to alloy, polar phonon, and charged impurity (concentration 10^{18} cm^{-3}) scattering.

Curves for a favorable alloy $Ga_{0.5}In_{0.5}As$ are shown in Fig. 4. The τ^{-1} curves now also include alloy scattering. Note that the mean free path for this alloy is about a factor of two greater than the corresponding ones for GaAs. However, the V_{gp} values are not much different in the two cases. Thus, if one plans to build devices with $L < \lambda_{GaAs}$ in any case, you might as well use the simpler GaAs material. However, if there is some problem that causes this to be impossible, one suffers no adverse consequences in V_g by choosing the alloy. Because the overshoot effect is still in doubt we quote in Table I only values of V_{gL} and λ_{gL} at the energy ϵ_L for electrons traveling in the 100 direction for several materials. Note that InAs is not a practical shoice since $\epsilon_g < \epsilon_L$ for this material.

Table I

	ϵ_L [meV]	V_{gL} [10^8 cm/s]	λ_{ϵ_L} [Å]
GaAs	300	1.09	1700
$Ga_{0.5}In_{0.5}As$	550	1.29	3720
InAs	790	1.38	7900
$Ga_{0.7}Al_{0.3}As$	125	0.75	486

As noted earlier there is little to be gained in V_{gL} by going to a hard-to-grow alloy, but there is a significant gain to be made in mean free path. Note also that $Ga_{0.7}Al_{0.3}$ As is significantly poorer than GaAs.

3. DRIFT DEVICES

Our major conclusions to date in this subject have already been published so we will only state the conclusions here. Under the influence of electric fields the conduction electrons are accelerated between collisions and their average energy increases until the energy relaxation decay rate equals the rate of energy gain from the field. When field strength reaches a level where the electron distribution becomes hot enough so significant numbers transfer from the high mobility central valley to the lower mobility satellite valley the drift velocity V_d reaches a peak V_{dp}.

At fields above this peak there is a region of negative differential resistance, followed by a region with a low positive slope finally ending at a saturated value. The peak drift velocity V_{dp} and the field $\mathcal{E}_{V_{dp}}$ are measures of device performance. For signal processing devices one wants V_{dp} as large as possible and $\mathcal{E}_{V_{dp}}$ to be small. We find that $Ga_{1-x}In_xAs$, $InP_{1-x}As_x$ and $InP_{1-x}Sb_x$ have characteristics superior to those of the compounds GaAs or InP.

4. CONCLUDING REMARKS

The theory of the transport properties of semiconductor alloys is approaching a level where it can be trusted as a materials screening tool for a variety of devide applications. When these results are coupled to the structural property calculations, growth models, fabrication models, and device modeling, one will have a generalized computer-aided design tool.

Acknowledgment

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